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PATHWAYS IN AN URBAN ENVIRONMENT**

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# POLLUTANT TRANSFER THROUGH AIR AND WATER PATHWAYS IN AN URBAN ENVIRONMENT

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## 1. INTRODUCTION

We are attempting to simulate the transport and fate of pollutants through air and water pathways in an urban environment. This cross-disciplinary study involves linking together models of mesoscale meteorology, air pollution chemistry and deposition, urban runoff and stormwater transport, water quality, and wetlands chemistry and biology. We are focusing on the transport and fate of nitrogen species because 1) they track through both air and water pathways, 2) the physics, chemistry, and biology of the complete cycle is not well understood, and 3) they have important health, local ecosystem, and global climate implications.

We will apply our linked modeling system to the Los Angeles basin, following the fate of nitrates from their beginning as nitrate-precursors produced by auto emissions and industrial processes, tracking their dispersion and chemistry as they are transported by regional winds and eventually wet or dry deposit on the ground, tracing their path as they are entrained into surface water runoff during rain events and carried into the stormwater system, and then evaluating their impact on receiving water bodies such as wetlands where biologically-mediated chemical reactions take place. In this paper, we wish to give an overview of the project and at the conference show preliminary results.

## 2. BACKGROUND

Several of the water bodies adjacent to Los Angeles have significantly elevated levels of pollutants (SMPRB, 1988). A few field experiments have shown that urban runoff in Los Angeles has elevated concentrations of nutrients, metals, and organic contaminants (Suffet et al., 1993; Wong et al., 1997). Wetlands are an effective mechanism for controlling the impact of non-point sources on receiving waters (Hey et al., 1994). Wetlands slow the flow of water thereby contributing to the settling of solids. Wetland

vegetation can assimilate nutrients and absorb heavy metals, and wetland soils can adsorb organic contaminants (Landers and Knuth, 1991). In So. California, many of the wetlands are in highly urbanized regions, and the flora and fauna in the related restoration projects may be deleteriously affected if the projects rely on runoff from urban land uses for the restoration of the hydrology (Helfield and Diamond, 1997).

Although urbanization of the LA basin is certainly responsible for much of their poor water quality, it is not certain exactly what sources are the major contributors. Similar to the initial phases of the Chesapeake Bay study (Jordan et al, 1991 and Fischer and Oppenheimer, 1997), it is not clear how significant atmospheric deposition is compared to urban runoff. In addition, the runoff itself contains some fraction of atmospherically-deposited pollutants. Several large-scale air quality studies in the Los Angeles basin have shown elevated levels of particulate pollution, including nitrates (e.g., Lawson, 1990, Russell et al., 1983, Solomon et al, 1992). With the modeling system described below, we will attempt to quantify the atmospheric contribution to the water quality problem and investigate the impacts of alternate wetlands strategies.

## 3. MODEL DESCRIPTIONS AND SET-UP

The system of linked models for studying the fate of pollutants through air and water pathways is shown in Fig. 1. In short, RAMS and HOTMAC will provide time-dependent 3-d meteorological fields to the CIT air chemistry code for wet and dry season cases, respectively. CIT will then simulate the gas and aerosol phase chemistry and produce wet and dry deposition fields of various pollutants. The deposited pollutants will be input to the SWMM model along with precipitation fields from RAMS. SWMM will compute urban runoff flow amounts and pollutant loading, which will then be utilized by the WASP model to simulate the fate of pollutants in a receiving water body. A short description of each model follows.

***RAMS (Regional Atmospheric Modeling System) and HOTMAC (Higher-Order Turbulence Model for Atmospheric Circulation).***  
RAMS (Pielke et al., 1992) and HOTMAC

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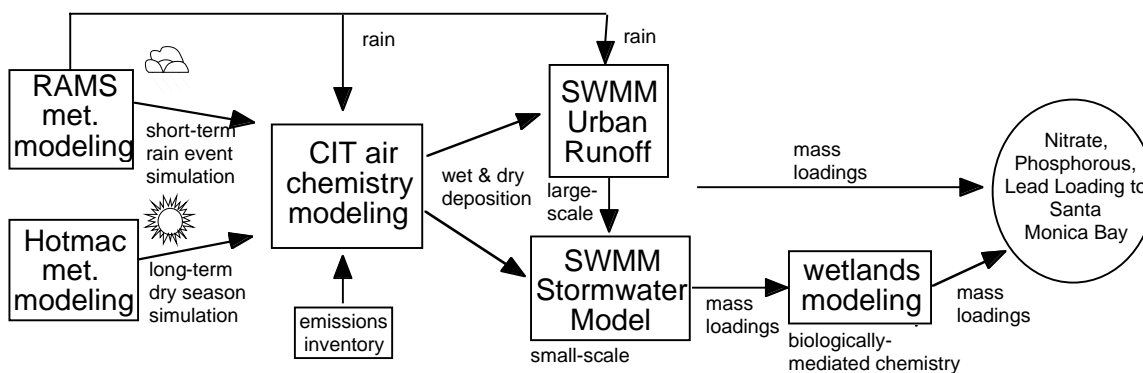


Figure 1. Modeling system for following pollutants through air-water pathways in an urban environment. With some modifications, the fate of pollutants from other sources could be modeled as well, for example accidental releases of toxic agents, heavy metals from brake pads, or noxious vapors from waste sites.

(Yamada and Kao, 1986) are both 3-d prognostic mesoscale meteorological models. Employing finite difference schemes, they solve the geophysical fluid dynamics conservation eqns. for mass, momentum, heat, and moisture, as well as thermal diffusion eqns. in the soil, a surface energy budget, and long and shortwave radiative fluxes.

For the wet weather simulations, RAMS will be run in non-hydrostatic mode and account for precipitation using a partial two moment microphysics scheme which includes eight water species. A nested grid approach using horizontal grid spacings of 80, 20, 5 and 1.25 km will be used in order to cover the synoptic scale weather over the Pacific Ocean and Western US and to resolve the region of interest, the LA basin (see Costigan, 1998). For the dry weather simulations, HOTMAC will be run in hydrostatic mode and use an urban canopy parameterization to account for the effect of sub-grid buildings. A 15, 5, and 1.67 km nested grid scheme is being used. The outer-most grid covers the lower 1/3 of California, the intermediate grid matches the CIT air chemistry domain, and the inner-most grid is centered over Santa Monica Bay effects (see Brown, 1998).

**CIT (Cal Tech/Carnegie Mellon) Air Chemistry Code.** The CIT airshed (chemistry-transport) model (McRae et al. 1982 and Russell et al. 1988) is a 3-d Eulerian photochemical model that solves the atmospheric diffusion equation using numerical methods. It uses the LCC (Lurmann, Carter, and Coyner) lumped molecule chemical mechanism and contains a resistance-based dry deposition module. The CIT model has not been formulated for wet deposition, so we will calculate total deposition of the soluble nitrogen species based on vertically-integrated column mass up to the model top at the time of the rainfall.

CIT will be applied to the Los Angeles basin for calculation of deposition of nitrogen-containing species for two periods during the 1987 Southern California Air Quality Study (SCAQS). The dry season simulation will be for August, 1987 and will use the SCAQS emission inventory and provide dry deposition and inferred buildup for the SWMM urban runoff model. Previously, CIT has been applied to the study of dry deposition of nitrogen species (NO, NO<sub>2</sub>, PAN, HNO<sub>3</sub>, NH<sub>3</sub>, and NH<sub>4</sub>NO<sub>3</sub>) in the Los Angeles basin for August, 1982 (Russell et al. 1993). 3-d meteorological fields will be supplied by the HOTMAC code.

The wet season simulation will be for an early December, 1987 episode in which high nitrate concentrations were noted. For this episode the RAMS model will be used to provide meteorological fields and precipitation. For both cases, the CIT model will have a single grid mesh with 5km resolution. The modeling domain is centered over the Santa Monica Bay watershed which includes 1,725 km<sup>2</sup> of the approximately 24,000 km<sup>2</sup> computational domain.

**SWMM (Storm Water Management Model).** For this project, SWMM (Huber and Dickinson 1988) has been selected to simulate the urban watershed and storm-sewer network. SWMM is a large, comprehensive software package capable of simulating the transport of precipitation and pollutants from the ground surface, through pipe/channel networks and storage/treatment facilities, and finally to receiving-waters. It is freely available from the USEPA.

Operationally SWMM is divided into computational and service "blocks". This study will use the RUNOFF Block of SWMM to simulate the transport of stormwater runoff and pollutants over the pervious and impervious surfaces of the urban watershed. The RUNOFF Block uses a non-linear

reservoir model for calculating runoff and empirically-derived build-up/ wash-off curves to estimate pollutant loading. Once the stormwater reaches a specified storm drainage inlet the TRANSPORT Block of SWMM is used to continue the simulation of the transport of runoff and pollutants through the storm drainage network. TRANSPORT uses the kinematic wave approximation (truncated St. Venant eqns.) for computing flow through pipes.

In this initial study, SWMM will operate on the output from a precipitation model (RAMS) and an atmospheric chemistry model (CIT) to drive the urban runoff simulation for a single rainfall event. For the RUNOFF Block, the Santa Monica and San Pedro Bay watersheds need to be divided into sub-catchments. Predominant land-use in each sub-catchment determines the build-up/ washoff expression to use. The TRANSPORT Block requires detailed pipe network information (inlet location, pipe size, slope, roughness). This Block will be used for Ballona, a subwatershed of Santa Monica Bay. The output from SWMM will be in the form of runoff hydrographs and pollutant-graphs describing the time-variable response of the urban area to the precipitation and deposition loading and will then be used as input to the wetlands modeling component.

**WASP (The Water Quality Analysis Simulation Program).** WASP5 (Ambrose et al., 1993) is a receiving water body contaminant fate and transport model. It is a dynamic compartment model utilizing equations based on the conservation of mass to determine the concentrations of chemical constituents from point of input to point of output. It can be applied in one, two, or three dimensions and treats a water body as a series of computational elements. Elements can be surface water, benthic porewater, surface of the benthos, or subsurface of the benthos. Environmental properties and chemical concentrations are considered spatially constant within segments.

The WASP program includes six transport mechanisms: advection and dispersion in the water column, advection and dispersion in the porewater, settling, re-suspension, and sedimentation of solids, and evaporation or precipitation. WASP is often connected to DYNHYD, a hydrodynamics program which simulates the movement of water. In DYNHYD, the temporal and spatial movements of water are followed using a series of mass balance equations. WASP has two supporting sub-models: TOX15 and EUTRO5. These models predict dissolved and sorbed chemical concentrations in the sediment and water column and predict the effects of nutrients and organic

matter on dissolved oxygen and phytoplankton dynamics. EUTRO simulates the transport and transformation reactions of up to eight state variables within four interacting systems: phytoplankton kinetics, the phosphorus cycle, the nitrogen cycle and the dissolved oxygen balance. EUTRO solves a mass balance equation adding specific transformation processes for the eight state variables in the water column and benthos. WASP inputs include advective and dispersive transport, boundary concentrations, point and diffuse source waste loads, kinetic parameters, constants and time functions, and initial concentrations. WASP5 does not simulate overland flow which is the main mechanism of non-point source pollution, but can use the output from a nonpoint source model, such as SWMM, as input.

The WASP model will be setup to cover the Ballona Wetland, a coastal saltmarsh and the historic drainage basin for the Ballona sub-watershed of Santa Monica Bay in Los Angeles, California. Pollutant loadings and inflow rates will be input from the SWMM model. Tidal information will be necessary for outflow boundary conditions. Several wetlands design criteria will be evaluated in terms of their impact on water quality.

#### 4. DISCUSSION

We have several goals for this project: the first is to integrate models for studying the urban environment; the second is to develop new sub-modules that account for the interface physics and feedback mechanisms between models; and the third is to contribute to the better understanding of the air-water nitrate pollution problem in the Los Angeles basin. Below, we will discuss several issues that have arisen due to the urban and cross-disciplinary nature of the problem.

Our study problem is pushing research development within individual models to deal with, for example, size-resolved aerosol chemistry and physics, aqueous phase air chemistry, biological mediation of water chemistry, fine resolution cloud and precipitation modeling, and urban canopy effects on meteorological fields. In addition, since the Santa Monica Bay watershed is not completely urbanized and contains mixed land, SWMM (developed to simulate urbanized areas) will need to be modified to account for non-urban runoff.

In addition, several feedback dynamics and interface issues between models need to be resolved, including the relationship between air chemistry production of secondary aerosols and meteorological production of clouds, the interaction of physical, chemical, and biological

components in the nitrogen cycle in water, the fate of particulates after they deposit on the ground, and the relationship between precipitation predictions, runoff amounts, and mass loading values.

Finally, data availability and validation issues have arisen, namely that long-term datasets are temporally and spatially sparse, while the relatively dense short-term datasets for air and water quality do not coincide in space and time and are few in number. The lack of water quality data is especially important for SWMM as the washoff algorithms require site-specific calibration data.

## 5. CONCLUSIONS

We have described a linked set of models that will be used for studying the transport and fate of pollutants through air and water pathways in an urban environment. Our first step involves manually inputting output from one model to another. Eventually, we will need to consider building models or sub-modules that account for interface physics and, if appropriate, feedback mechanisms.

Our ultimate goal for this project is to link together other models of urban infrastructure and natural systems in order to understand the complex interactions of the urban and natural environments. Such a modeling system could be used for urban planning, sustainability studies, and vulnerability assessment. More information on other work ongoing in this project can be found at <http://geont1.lanl.gov/urbansecurity.htm>.

## 6. REFERENCES

- Ambrose, R., T. Wool, J. Martin, "The Water Quality Analysis Simulation Program, WASP5, Part A: Model documentation, Version 5.10." USEPA, Env. Research Lab., Athens, GA (1993).
- Brown M., "Meteorological modeling in the Los Angeles basin using a modified urban canopy parameterization," AMS 2<sup>nd</sup> Urban Env. Symp., Albuquerque, NM (1988).
- Costigan K., "Simulation of a winter precipitation event for Los Angeles water quality studies," AMS 2<sup>nd</sup> Urban Env. Symp., Albuquerque, NM (1988).
- Fisher, D and Oppenheimer, M., "Atmospheric nitrogen deposition and the Chesapeake Bay Estuary." *Ambio*, 20: 102-108 (1991).
- Huber W. and R. Dickinson. "Storm Water Management Model, Version 4: Part A, User's Manual." EPA-600/3-88-001a, USEPA, Washington, DC. (1988).
- Jordan T., Correll, D., and Weller, D., "Nonpoint source discharges of nutrients from Piedmont watersheds of Chesapeake Bay." *J Amer. Water Resources Assoc.*, 33(3): 631-645 (1997).
- Helfield, J.M. and M.L. Diamond. 1997. Use of constructed wetlands for urban stream restoration: a critical analysis. *Environmental Management* 21 (3): 329-341.
- Hey, D., A. Kenimer, and K. Barrett, "Water quality improvement by four experimental wetlands," *Ecological Engineering* 3, 381-397 (1994.).
- Landers, J. and B. Knuth, "Use of wetlands for water quality improvement under the USEPA Region V Clean Lakes Program," *Environmental Management* 15 (2): 151-162 (1991).
- Lawson D., "Southern California Air Quality Study," *JAPCA* 40 (1990).
- McRae G., W. Goodin and J. Seinfeld. *Atmos. Environ.* 16, 679-696 (1982).
- Pielke R., W. Cotton, R. Walko, C. Tremback, W. Lyons, L. Grasso, M. Nicholls, M. Moran, D. Wesley, T. Lee, and J. Copeland, "A Comprehensive Meteorological Modeling System", *Meteorol. Atmos. Phys.* 49, 69-91 (1992).
- Russell A., K. McCue, and G. Cass, *Environ. Sci. Technol.* 22, 263-271 (1988).
- Russell A., D. Winner, R. Harley, K. McCue, and G. Cass, "Mathematical modeling and control of the dry deposition flux of nitrogen-containing air pollutants," *Environ. Sci. Technol.* 27, 2772-2782 (1993).
- Solomon P., L. Salmon, T. Fall, and G. Cass, "Spatial and temporal distribution of atmospheric nitric acid and particulate nitrate concentrations in the Los Angeles area," *Environ. Sci. Tech.* 26, 1594-1601 (1992).
- SMPB, "Taking the Pulse of the Bay - State of the Bay 1998," Santa Monica Bay Restoration Project (April 1998).
- Suffet, I., J. Froines, E. Ruth, L. Schweitzer, and M. Capangpangan, "Chemical Contaminant Release into Santa Monica Bay: A Pilot Study," Final Report, Amer. Oceans Campaign (1993).
- Wong, K., E. Strecker, and M. Stenstrom, "GIS to estimate storm-water pollutant mass loadings," *J Env. Eng.*, 737-745 (1997).
- Yamada T. and J. Kao, "A modeling study on the fair weather marine boundary layer of the GATE," *J. Atm. Sci.* 43, 3186-3199 (1986).